Fourth Order Compact Implicit Method for the Maxwell Equations with Discontinuous Coefficients

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Abstract

We consider fourth order accurate compact schemes for numerical solutions to the Maxwell equations. The same mesh stencil is used as in the standard Yee scheme. In particular extra information over a wider stencil is not required. This has several advantages. First, it is relatively easy to modify an existing code based on the Yee algorithm to make it fourth order accurate. Second, a staggered mesh, without additional mesh locations, makes the boundary treatment easier since some of the quantities are located inside the domain rather than on the boundary. Also, a staggered grid system gives a lower error than a similar non-staggered system. The extension to dielectric materials is presented. This uses a compact implicit smoothing operator to redefine the piecewise constant dielectric coefficients.

1 Maxwell Equations

We consider the TM system. We nondimensionalize the time. Let $\tau = ct = t/\sqrt{\mu\epsilon}$ and $Z = \sqrt{\frac{\mu}{\epsilon}}$, where ϵ and μ are the permittivity and permeability coefficients, in free space, respectively and c is the speed of light. The TM wave equations then become:

$$\begin{aligned}
\frac{\partial E_z}{\partial \tau} &= Z(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}) \\
\frac{\partial H_x}{\partial \tau} &= -\frac{1}{Z}\frac{\partial E_z}{\partial y} \\
\frac{\partial H_y}{\partial \tau} &= \frac{1}{Z}\frac{\partial E_z}{\partial x}
\end{aligned} \tag{1}$$

2 Finite Differences Scheme

We present Yee's difference equations in a form that will enable us to generalize them easily.

$$
\begin{aligned}
E^{n+1}_{z,i,j} &= E^{n}_{z,i,j} + Z\frac{\Delta\tau}{\Delta x}\delta_x H^{n+1/2}_{y,i,j} - Z\frac{\Delta\tau}{\Delta x}\delta_y H^{n+1/2}_{x,i,j} \\
H^{n+1/2}_{x,i,j-1/2} &= H^{n-1/2}_{x,i,j-1/2} - \frac{1}{Z}\frac{\Delta\tau}{\Delta y}\delta_y E^{n}_{z,i,j-1/2} \\
H^{n+1/2}_{y,i-1/2,j} &= H^{n-1/2}_{y,i-1/2,j} + \frac{1}{Z}\frac{\Delta\tau}{\Delta x}\delta_x E^{n}_{z,i-1/2,j}
\end{aligned}
\tag{2}
$$

where
Yee:

$$
\begin{aligned}
\delta_x U_{i,j} &= U_{i+1/2,j} - U_{i-1/2,j} \\
\delta_y U_{i,j} &= U_{i,j+1/2} - U_{i,j+1/2}
\end{aligned}
\tag{3}
$$

U is evaluated at the appropriate time and space location.

In order to improve the accuracy of the scheme we replace (3) by an implicit scheme. We approximate the spatial derivatives to fourth order, using the following implicit method for $\frac{\partial U}{\partial y}$:
Ty(2,4):
Define

$$
\mathbf{A} = \frac{\mathbf{1}}{\mathbf{24}}\begin{pmatrix}
26 & -5 & 4 & -1 & . & . & 0 \\
1 & 22 & 1 & 0 & . & . & 0 \\
0 & 1 & 22 & 1 & 0 & . & 0 \\
. & . & . & . & & & \\
0 & . & . & 0 & 1 & 22 & 1 \\
0 & . & . & -1 & 4 & -5 & 26
\end{pmatrix}.
$$

The matrix form of these approximations is:

$$
\mathbf{A}\frac{\partial}{\partial \mathbf{y}}\begin{bmatrix} U^{1/2} \\ U^{3/2} \\ . \\ . \\ U^{(2p-1)/2} \end{bmatrix} = \frac{\mathbf{1}}{\Delta \mathbf{y}}\left(\begin{bmatrix} U^{1} \\ U^{2} \\ . \\ U^{p-1} \\ U^{p} \end{bmatrix} - \begin{bmatrix} U^{0} \\ U^{1} \\ . \\ U^{p-2} \\ U^{p-1} \end{bmatrix}\right). \tag{4}
$$

A similar formula holds for other variables shifted to other locations and in each direction. We stress that the only difference between the Yee scheme and the (2,4) scheme is the multiplication by A^{-1}. A^{-1} is never evaluated, but rather the decomposition $A = LU$ is calculated once in each direction. L and U are bidiagonal matrices with one of them having "ones" along the diagonal. The scheme is fourth order in space but only second order in time. This is a reasonable option since we can improve the temporal accuracy by choosing a smaller time step. This increases the work only linearly and does not increase the storage. A fourth order scheme in space enables us to choose a coarser mesh. This decreases the work in each space dimension and also decreases the storage. Hence, the accuracy in space is of greater importance then the accuracy in time. As a consequence one should choose a time step based on accuracy conditions and not on stability grounds, [3].

Another option is to replace the leapfrog scheme by a fourth order Runge-Kutta scheme. The resultant scheme is fourth order accurate in both space and time. With this scheme the variables are staggered in space but not in time. One then has a choice of several versions of a fourth order Runge-Kutta scheme. One possibility is to use the classical scheme. A further improvement can be achieved by using the higher resolution fourth order Runge-Kutta scheme proposed by Hu et. al. [5].

For a linear set of equations we can simplify the classical Runge-Kutta system for $\frac{\partial U}{\partial t} = f(U)$ to

$$\begin{aligned} U^{(1)} &= U^n + \frac{\Delta t}{4} f(U^n) \\ U^{(2)} &= U^n + \frac{\Delta t}{3} f(U^{(1)}) \\ U^{(3)} &= U^n + \frac{\Delta t}{2} f(U^{(2)}) \\ U^{n+1} &= U^n + \Delta t f(U^{(3)}) \end{aligned} \tag{5}$$

Although this scheme is only second order for general function f, nevertheless it is fourth order for linear functions f as occur in the Maxwell equations. One needs to store U^n and the last iterate of U throughout the grid. One can store f throughout the grid or else calculate it along each line and then update so that f is only stored along a single direction. Thus, effectively only two storage locations are required for the electric and magnetic fields.

Boundary conditions are imposed at the end of the leapfrog step or the end of each stage of the Runge-Kutta method. At solid boundaries the method was chosen so that the same technique used for the Yee scheme can still be used for the fourth order method, see also [12].

In the far field we use the PML technique [2, 10]. An important feature of the PML system is that the only spatially differentiated terms are the physical variables. Hence, we can calculate all derivatives by the implicit method across the entire domain including both the interior and PML layers. Once the spatial derivatives are approximated we can advance each system in time independently both in the interior and in the PML layer.

2.1 Time Step

The amplification factor of the leapfrog and the RK schemes is given by:

$$\sigma = \begin{cases} 1 + \frac{1}{2}z^2 \pm \sqrt{(1+\frac{1}{2}z^2)^2 - 1} & \text{leapfrog} \\ 1 + z + \frac{1}{2}z^2 + \frac{1}{6}z^3 + \frac{1}{24}z^4 & \text{RK-4} \end{cases}$$

$z = \lambda \Delta t$ where λ is an eigenvalue of the Fourier transform of the spatial approximation. Let $D = \left[\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2}\right]^{1/2}$. Then

$$|\lambda_{Yee}| = 2\left[\frac{\sin^2(\frac{\theta}{2})}{(\Delta x)^2} + \frac{\sin^2(\frac{\phi}{2})}{(\Delta y)^2}\right]^{1/2} \le 2D$$

$$|\lambda_{Ty}| = 24\left[\frac{\sin^2(\frac{\theta}{2})}{((\Delta x)(11+\cos(\theta)))^2} + \frac{\sin^2(\frac{\phi}{2})}{((\Delta y)(11+\cos(\phi)))^2}\right]^{1/2}$$

$$\le 2.4D$$

Define $\mathbf{CFL} = \frac{\Delta t}{\Delta x}$ then for stability we have to choose:

$$\begin{aligned} CFL_{Yee} &\le \frac{1}{\sqrt{2}} \\ CFL_{Ty(2,4)} &\le \frac{1}{1.2\sqrt{2}} \\ CFL_{Ty(4,4)} &\le \frac{5}{6}. \end{aligned}$$

2.2 Numerical Errors of Spatial and Time Discretization

We now investigate the numerical errors from the combined discretization. These errors can be determined from the eigenvalues of the amplification matrix. In Fig. 1 the curves labeled 'exact' are the normalized phase shift using the exact time integration. The difference between these curves and the value 1 is the spatial phase error, which can either be a phase lag or a phase lead. The other curves are the normalized phase shift using the staggered leapfrog and RK-4 (with Yee and Ty) with **CFL** $= \frac{1}{2}$. For the Yee scheme the difference between each curve and the exact curve is an additional phase error due to time discretization. Although this additional phase error is small for RK-4 it moves the curve further away from 1 because both have a phase lag. For the Ty scheme both RK-4 and the exact curves are closer to 1 and experiences a phase lag. Leapfrog has a larger error and a phase lead and so moves the curve away from 1 which makes the total error larger than with RK-4. Except for a very small contribution due to the nonlinear relation between σ and λ, the time discretization does not reduce the isotropy error introduced by the spatial discretization.

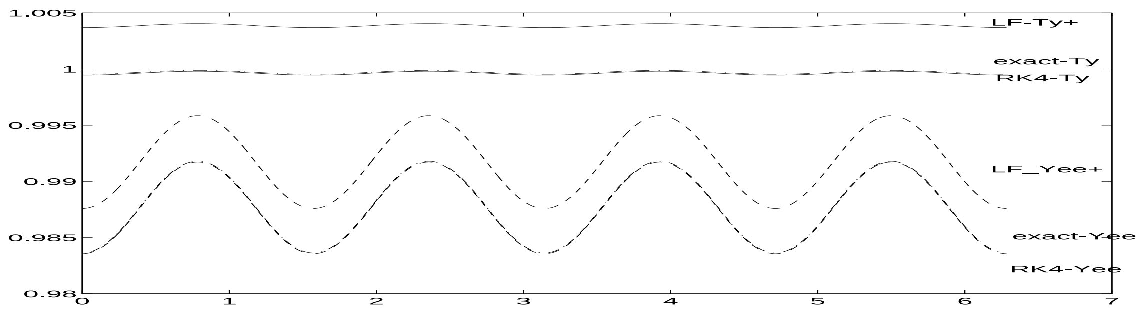

Figure 1: Comparison of phase shifts for complete discretization.

3 Dependence of Accuracy On CFL

We next consider the Maxwell equations in free space, in two dimensions, with boundary conditions

$$
\begin{aligned}
E_z(0,y,t) &= -\sin(4\pi t) + \sin(4\pi(y-t)) \\
E_z(x,0,t) &= \sin(4\pi(x-t)) - \sin(4\pi t) \\
H_y(h/2,y,t) &= \sin(4\pi(h/2-t)) \\
H_x(x,h/2,t) &= \sin(4\pi(h/2-t))
\end{aligned} \tag{6}
$$

The exact solution is $E_z = \sin(4\pi(x-t)) + \sin(4\pi(y-t))$. We choose $h = \Delta x = \Delta y = 1/40$ and $\Delta t = 1/80, 1/160, ..., 1/1200$. Hence, the **CFL** numbers range from 1/2 to 1/30.

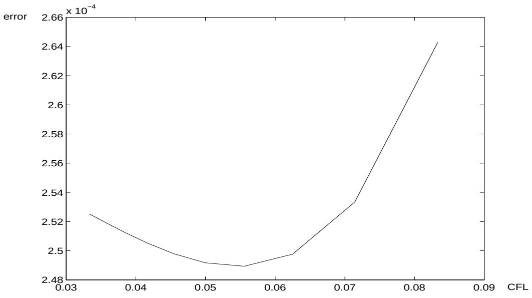

Figure 2: The error for (6) with Ty2,4. Δt varies from $\frac{h}{30}$ to $\frac{h}{10}$.

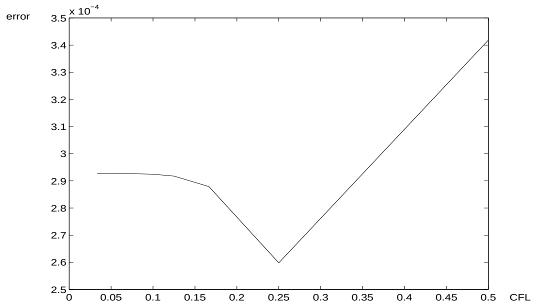

Figure 3: The error with Ty4,4 as Δt varies from $\frac{h}{30}$ to $\frac{h}{10}$.

In figure 2 one sees that the minimal error in Ty(2,4) occurs at $CFL = \frac{1}{18}$. This corresponds to the error in the phase shift being minimal at $CFL = \frac{1}{18}$. In Fig. 3 we see that the minimal error for Ty(4,4) occurs at $CFL = \frac{1}{4}$. To compare Yee's scheme with Ty we choose $\Delta x = \Delta y = h$ and $\Delta t = \frac{2}{3}h$ where h= 1/80, 1/120, 1/160, 1/240, 1/280, 1/320, 1/360. When $h = 1/360$ the error for Yee's scheme is comparable to the error for Ty(2,4) with $h = 1/40$, $\Delta t = 1/160$ (see figure 4). In Fig. 5, we plot the log of the error as a function of log(h).

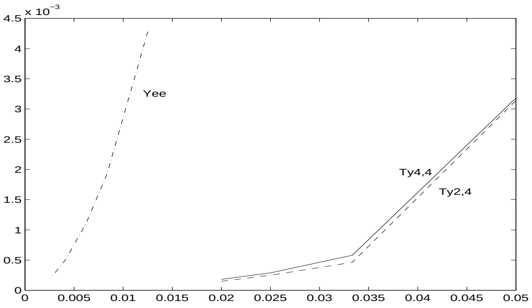

Figure 4: The error as h varies from $\frac{1}{360}$ to $\frac{1}{80}$ for Yee and $\frac{1}{50}$ to $\frac{1}{20}$ for Ty.

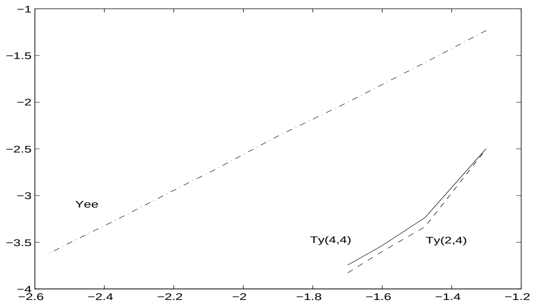

Figure 5: Logarithm of the error as a function of log(h). h varies from $\frac{1}{360}$ to $\frac{1}{20}$ for Yee and $\frac{1}{50}$ to $\frac{1}{20}$ for Ty.

4 Computational Results

We now compare the efficiency of three different schemes: the standard Yee scheme, the (2,4) scheme advanced in time by a leapfrog method and the (4,4) scheme advanced in time by a Runge-Kutta scheme. For conciseness of notation we shall refer to these schemes as Yee, Ty(2,4) and Ty(4,4) respectively. For all computations we choose $Z = 1$. All the cases use a PML layer in the far field [10].

We first consider a monochromatic isotropic point source of wavelength 0.25, that is switched on at $t = 0$. The domain is $0 \leq x, y \leq 0.9$. For Yee's scheme we choose $h = \frac{1}{160}$, $\Delta t = \frac{2h}{3} = \frac{1}{240}$, for Ty(4,4): $h = \frac{1}{20}$, $\Delta t = \frac{h}{4} = \frac{1}{80}$ while for Ty(2,4) $h = \frac{1}{20}$, $\Delta t = \frac{h}{18} = \frac{1}{360}$. The point source is modeled by adding a term representing a current $I_z(t) = 0.01 \sin(8\pi t)\epsilon(t)$ at $(x, y) = (\frac{1}{5}, \frac{1}{5})$ where $\epsilon(t)$ denotes the Heaviside unit-step function. For the pulse under consideration, the radiated field is the solution of

$$\partial_x^2 E_z + \partial_y^2 E_z - \partial_t^2 E_z = Z \partial_t I_z(t) \delta(r - r_s) \tag{7}$$

$r - r_s = (x - \frac{1}{5}, y - \frac{1}{5})$. The solution consists of rotationally symmetric outgoing waves. The exact solution is

$$E_z(r, t) = -\frac{Z}{2\pi} \int_0^\infty \frac{\partial_t \boldsymbol{I_z(t - \sqrt{|(r - r_s|^2 + \xi^2})}}{\sqrt{|(r - r_s|^2 + \xi^2}} d\xi$$

In Fig. 6 we display the exact solution on the line $y = x$. In Fig. 7 we plot the errors, in the L_2 norm, for the various approximate solutions.

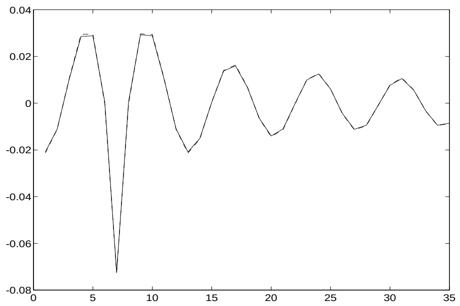

Figure 6: Solution of (7) on the line $y = x$ after 320 time steps.

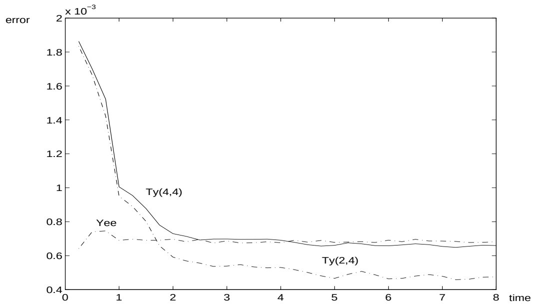

Figure 7: The errors in the numerical solution of (7).

We next consider the propagation in a rectangular cross section wave guide. We take the walls to be perfect conductors. Boundary and initial conditions are

$$E_z(x, 0, t) = \sin(4\pi x) \sin(-5\pi t)$$
$$E_z(1, y, t) = 0 \quad E_z(0, y, t) = 0.$$

The solution is then:

$$E_z(x, y, t) = \sin(4\pi x) \sin(3\pi y - 5\pi t).$$

We choose the same grid as for the pulse. We get similar accuracy for the various schemes with this choice of meshes. In Fig. 8 we plot the error for the Yee and Ty schemes as a function of time. For the Yee scheme the error is computed every 4 time steps and for the Ty scheme every 5 time steps. These results demonstrate that we can use a much coarser mesh with the fourth order scheme and still get the same accuracy as with the Yee scheme. A factor of 8 in the mesh in each direction translates into a factor of 64 in work for a two dimensional problem and 512 in three dimensions. Because of the coarser mesh the (2,4) scheme uses a time step only one third smaller than the Yee scheme. This more than compensates for the extra time required by the scalar tridiagonal inversions. This is even more important in three space dimensions.

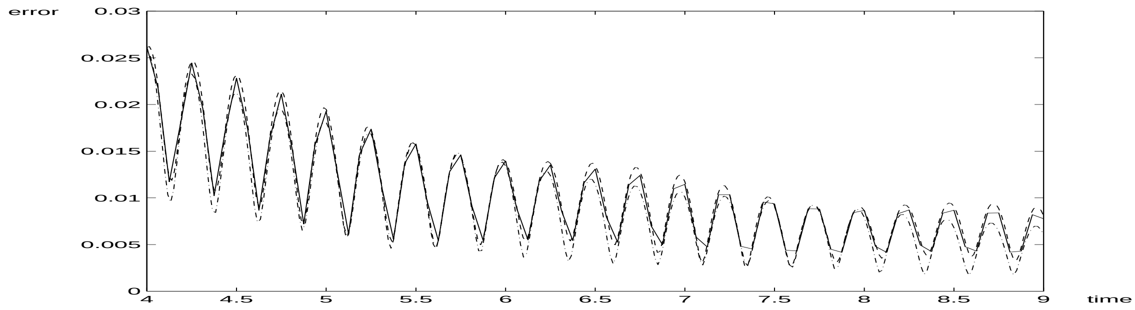

Figure 8: The errors for the waveguide: Ty(2,4), Ty(4,4) coincide. Yee is drawn by $-.-$.

Next consider a domain containing a lossless dielectric in the domain $|x| \leq \frac{1}{2}$ with a relative permittivity of $\epsilon = 4, \mu = 1$ (see Fig 9):

$$\begin{aligned}
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}\left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right) \\
\frac{\partial H_x}{\partial t} &= -\frac{1}{\mu}\frac{\partial E_z}{\partial y} \\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}\frac{\partial E_z}{\partial x}
\end{aligned}$$

The exact solution is:

$$E_z = \begin{cases} 2\cos(\frac{2\pi}{3}X)\cos(\omega t)\sin(K_y Y) & |X| \leq \frac{1}{2} \\ & 0 \leq Y \leq 1 \\ \exp(\frac{\pi\sqrt{3}}{3})\exp(-\frac{2\pi\sqrt{3}}{3}|X|)\cos(\omega t)\sin(K_y Y) & |X| \geq \frac{1}{2} \\ & 0 \leq Y \leq 1 \end{cases}$$

Where

$$
\begin{aligned}
K_y &= \sqrt{\frac{13}{3}}\frac{2\pi}{3} \\
\omega &= \frac{4\pi}{3\sqrt{3}}
\end{aligned}
$$

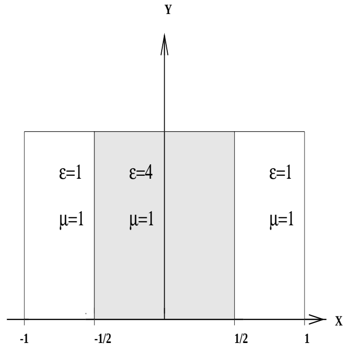

Figure 9: The computational domain

An arithmetic average of ϵ at the interface reduces the accuracy to second order. Instead we use an implicit fourth order interpolation to define $\epsilon_{i,j}$ at the nodal points.

$$
\frac{1}{8}\begin{bmatrix} 10 & -5 & 4 & -1 & . & . & 0 \\ 1 & 6 & 1 & 0 & . & . & 0 \\ 0 & 1 & 6 & 1 & 0 & . & 0 \\ . & . & . & . & & & \\ 0 & . & . & 0 & 1 & 6 & 1 \\ 0 & . & . & -1 & 4 & -5 & 10 \end{bmatrix} \begin{bmatrix} \frac{1}{\epsilon_1} \\ \frac{1}{\epsilon_2} \\ . \\ \frac{1}{\epsilon_{p-2}} \frac{1}{\epsilon_{p-1}} \end{bmatrix}
$$

$$
= 0.5\left(\begin{bmatrix} \frac{1}{\epsilon_{3/2}} \\ \frac{1}{\epsilon_{5/2}} \\ . \\ \frac{1}{\epsilon_{p-\frac{3}{2}}} \\ \frac{1}{\epsilon_{p-1/2}} \end{bmatrix} + \begin{bmatrix} \frac{1}{\epsilon_{1/2}} \\ \frac{1}{\epsilon_{3/2}} \\ . \\ \frac{1}{\epsilon_{p-\frac{5}{2}}} \\ \frac{1}{\epsilon_{p-\frac{3}{2}}} \end{bmatrix}\right).
$$

In two dimensions this is replaced by

$$
\left(I + \frac{h^2}{8}\Delta\right)\epsilon_{ij} = \frac{\epsilon_{i+1/2,j+1/2} + \epsilon_{i-1/2,j+1/2} + \epsilon_{i+1/2,j-1/2} + \epsilon_{i-1/2,j-1/2}}{4}
$$

where the Laplacian is replaced by the standard central difference formula. This can be simply approximated by an ADI formula or else quickly solved by multigrid. In any case this requires only a preprocessing stage and so is done only once per calculation.

To compare the efficiency of the schemes we refine the mesh for the Yee scheme. We choose $\Delta x = \Delta y = 1/160$, $\Delta t_{Yee} = 1/240$ for the Yee scheme. For the Ty(2,4) and Ty(4,4) schemes we choose $\Delta x = \Delta y = 1/20$, $\Delta t_{Ty(2,4)} = 1/360$, $\Delta t_{Ty(4,4)} = 1/80$. We now get comparable errors for all the schemes (see Fig(10)). Thus, even in the presence of a dielectric media we can choose a mesh that is eight times coarser in each direction for the fourth order schemes and still achieve errors that are smaller than that of the second order Yee scheme.

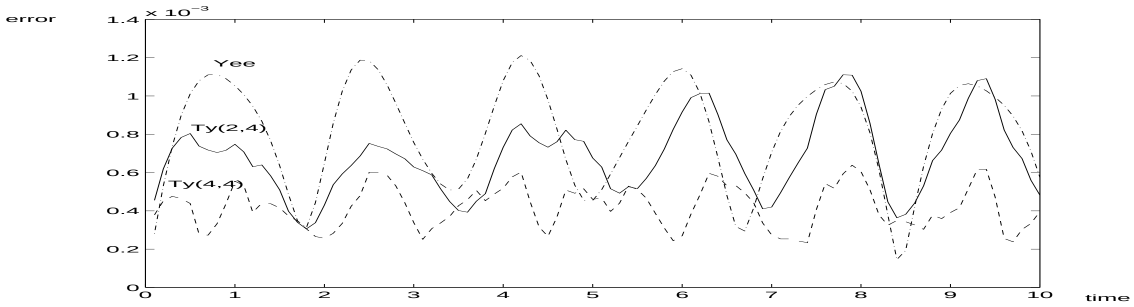

Figure 10: Dielectric: Yee is drawn by $-.$, Ty(2,4) by a solid line and Ty(4,4) by $--$.

We conclude that both fourth order methods are much more accurate and efficient than Yee's scheme. Yee requires a mesh about 8 times finer in each direction than the staggered fourth order scheme to achieve similar accuracy. The accuracy of the (2,4) and (4,4) schemes can be made comparable by choosing an appropriate time step. For the (4,4) scheme $CFL = \frac{1}{4}$ seems to be optimal. Since this is a four stage method it is equivalent to $CFL = \frac{1}{16}$ per stage. For the (2,4) scheme the time step needs to be chosen smaller the greater the accuracy one desires. Here $CFL = \frac{1}{18}$ was found best. Thus, the (2,4) is only slightly less efficient than the (4,4) scheme. The major advantage of the (2,4) scheme is that it requires less programming if one already has an existing code based on the Yee algorithm. Also, the (2,4) algorithm is non-dissipative while the (4,4) Runge-Kutta scheme introduces a slight dissipation. So each one has its advantages depending on the application.

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